

## **Chapter – 4**

### **INNOVATIVE METHOD FOR THE PREDICTION OF THE BOND ORDER OF DIATOMIC SPECIES WITHOUT MOLECULAR ORBITAL THEORY (MOT)**

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In the previous chapters 1 & 2, formulae-based mnemonics have been discussed to predict the power of the hybridization state of simple molecules or ions, carbon atoms in organic compounds and heteroatom in the heterocyclic compounds. Limitations of conventional formula have been focused in chapter 3 in the light of innovative formulae. In this chapter-4, bond order of diatomic species having the total number of electrons (1-20), has been predicted without drawing a molecular orbital diagram or without using molecular orbital theory. Here, I have tried to hub four (04) time economic innovative mnemonics by including four (04) formulae to predict the bond order of diatomic species. Here, I have also discussed the application of bond order in chemical bonding and different problems associated with it. This chapter explores the results and gives implications for context-based teaching, learning, and assessment.

Bond-order usually predicted from the Molecular Orbital Theory. Molecular Orbital Theory (M.O.T.) was first proposed by Friedrich Hund and Robert Mulliken in 1933<sup>1,2</sup>. They developed an approach to the covalent bond formation which is based upon the effects of the various electron fields upon each other and which employs molecular orbital rather than atomic orbital. Each such orbital characterizing the molecule as a whole is described by a definite combination of quantum numbers and possesses relative energy value.

#### **METHODOLOGY**

##### **A. The conventional method for prediction of bond order with molecular orbital theory (MOT)**

Molecular orbital theory (MOT), was proposed by Hund and Mulliken in 1933. According to this theory, in a molecule, formation all atomic orbitals of participating atoms overlap or mix up to form the equivalent number of new orbitals called molecular orbitals. In doing so, the atomic orbitals lose their individual identity and all the electrons get distributed in molecular orbital in accordance with Aufbau's principle, Paulis exclusion principle and Hund's rule.

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1. R S. Mulliken, *Spectroscopy, Molecular Orbitals, and Chemical Bonding Nobel Lectures Chemistry* (Amsterdam Elsevier Publishing Company:1972),1963-1970.

2.George G. Hall, "The Lennard-Jones Paper of 1929 and the foundations of Molecular Orbital Theory", *Advances in Quantum Chemistry* 22 (1991): 1-6, doi:10.1016/S0065-3276(08)60361-5.

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Formation of molecular orbitals explained on the basis of the linear combination of atomic orbitals (LACO). When atomic orbitals approach each other, their wave functions ( $\psi$ ) interact with each other in two different ways:

**i) Bonding molecular orbital (BMO):** Constructive interference i.e. when two waves are in phase and produce an additive effect to give rise to bonding molecular orbital (BMO).

**ii) Antibonding molecular orbital (ABMO):** Destructive interference i.e. when two waves are out of phase and produce the subtractive effect to give rise to antibonding molecular orbital (ABMO).

Bonding molecular orbitals (BMOs) are formed by the addition of atomic orbitals and are represented by  $\sigma$ ,  $\pi$  etc.. Energy of BMOs is lower than that of combining atomic orbitals. Antibonding molecular orbitals (ABMOs) are formed by subtraction of atomic orbitals and are represented by  $\sigma^*$ ,  $\pi^*$  etc.. Energy of ABMOs is higher than that of combining atomic orbitals. ABMOs are higher in energy than the corresponding BMOs. Thus, BMOs are more stable than ABMOs. Electrons first enter in lower energetic BMO by obeying Hund's rule then enters in corresponding higher energetic ABMO. The probability of finding electrons, increases in BMO, whereas, decreases in ABMO.

The atomic orbitals, which do not take part in bond formation, are known as non-bonding orbitals. Ex. In HF, sigma bonding and antibonding orbitals are formed by combining 1s orbital on H-atom with the  $2p_z$  orbital on fluorine (F) atom. This is why, 1s, 2s,  $2p_x$  and  $2p_y$  orbitals on fluorine (F) remain as nonbonding orbitals.

#### Increasing energetic order of different molecular orbitals for number of electrons $\leq 14$

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2p_x} = \pi_{2p_y} < \sigma_{2p_z} < \pi^*_{2p_x} = \pi^*_{2p_y} < \sigma^*_{2p_z}$$

#### Increasing energetic order of different molecular orbitals for number of electrons $> 14$

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \sigma_{2p_z} < \pi_{2p_x} = \pi_{2p_y} < \pi^*_{2p_x} = \pi^*_{2p_y} < \sigma^*_{2p_z}$$

In this energetic order, there is five bonding molecular orbitals (BMOs),  $\sigma_{1s}$ ,  $\sigma_{2s}$ ,  $\pi_{2p_x}$ ,  $\pi_{2p_y}$ ,  $\sigma_{2p_z}$  and five anti bonding molecular orbitals (ABMOs),  $\sigma^*_{1s}$ ,  $\sigma^*_{2s}$ ,  $\pi^*_{2p_x}$ ,  $\pi^*_{2p_y}$ ,  $\sigma^*_{2p_z}$ .

**iii) Bond Order (B.O.):** The number of covalent bonds formed in a molecule is called its bond order.

**Mathematically, it is represented as**  $B.O. = N_b - N_a / 2$ ,

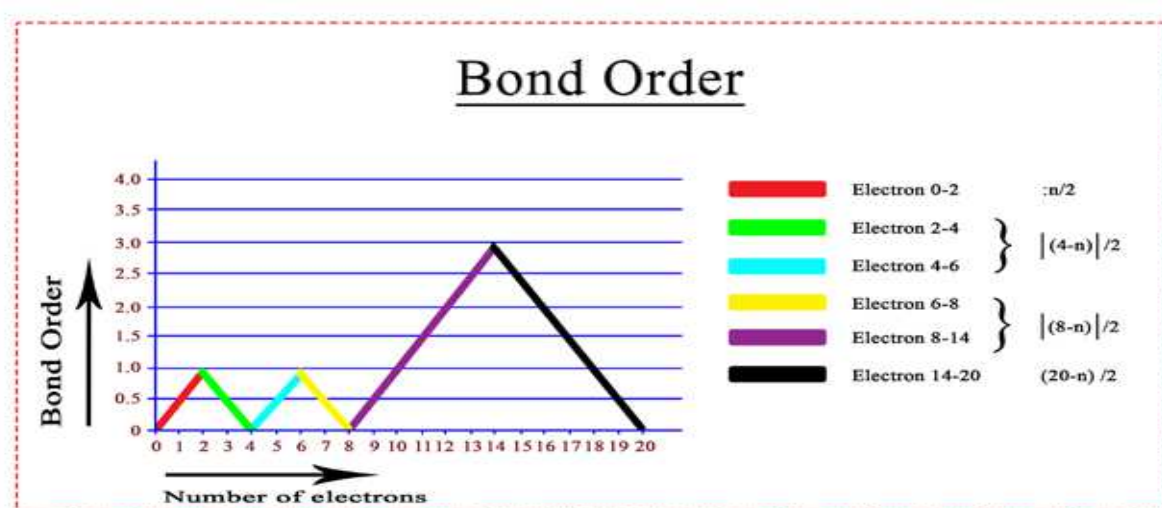
Where,  $N_b$  = Number of electrons in bonding molecular orbitals,  $N_a$  = Number of electrons in anti bonding molecular orbitals.

If,  $N_b > N_a$ , then B.O. = +ve, the molecule is stable and if,  $N_b < N_a$ , then B.O. = -ve, the molecule is unstable or does not exist. If,  $N_b = N_a$ , B.O. = 0, the molecule does not exist.

## B. Innovative Method for the prediction of bond order without molecular orbital theory

First of all, classify the molecules or ions having (1-20)e<sup>-</sup>s into the following four (4) types, (1-2), (2-6), (6-14) and (14-20), based on the total number of electrons present in them.

The graphical representation (**Fig.4.21**), shows that bond-order gradually increases to 1 in the range (0-2) electrons, then falls to zero in the range (2-4) electrons, then it further rises to 1 for (4-6) electrons and once again falls to zero for (6-8) electrons, then again rises to 3 in the range (8-14) electrons and then finally falls to zero for (14-20) electrons. For total no of electrons 2, 6 and 14, one can use multiple formulae, because they fall in the overlapping region in which they intersect with each other.



**Fig.4.21: Graphical Representation of B.O. with the number of electrons**

For such four divisions based on the total number of electrons, there will be four formulae to predict bond order of homo and heteronuclear diatomic molecules or ions having the total number of electrons fall in the range (1-20)<sup>3-8</sup> as follows:

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3. A. Das, "Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory", *World Journal of Chemical Education* 5 (June 2017):128-131, doi: 10.12691/wjce-5-4-2, <http://pubs.sciepub.com/wjce/5/4/2/>.
  4. A. Das, "Innovative Mnemonics in Chemical Education - A Review Article", *American Journal of Chemistry and Applications* 5(April 2018): 19-32, <http://www.openscienceonline.com/journal/archive2?journalId=711&paperId=4221>.
  5. A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education", *International Journal of Physics & Chemistry Education* 10 (June 2018):27-40, doi: 10.12973/ijpce/81589, <http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html>.
  6. A. Das, "Innovative Mnemonics In Chemical Education: Review Article", *African Journal of Chemical Education* 8(July 2018):144-189, <https://www.ajol.info/index.php/ajce/article/view/176086>.
  7. A. Das, "Innovative Mnemonics Make Chemical Education Time Economic – A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018):154-174, doi:10.12691/wjce-6-4-2, <http://pubs.sciepub.com/wjce/6/4/2/index.html>.
  8. A. Das, "Chemical Bonding: Time Economic Innovative Pedagogies - A Review Article", *Global Journal of Science Frontier Research Chemistry* 17 (Nov 2017): 1-16, <https://journalofscience.org/index.php/GJSFR/article/view/2110>.

**i) Molecules and ions having total no of electrons within the range (1-2):**

In such case Bond order =  $n/2$

**ii) Molecules and ions having total no of electrons within the range (2-6):**

In such case Bond order =  $(4 - n) / 2$

**iii) Molecules and ions having total no of electrons within the range (6-14):**

In such case Bond order =  $(8 - n) / 2$

**iv) Molecules and ions having total no of electrons within the range (14-20):**

In such case Bond order =  $(20 - n) / 2$

[where,  $n$  = Total no of electrons, 'II' indicates Mod function i.e. the value of bond order is always positive]

In the above formulae by just putting the value of the total number of electrons ( $n$ ), bond order of diatomic species should easily be predicted without using molecular orbital theory (MOT).

**RESULTS AND DISCUSSION****A. Prediction of bond order by conventional method:**

By using conventional method bond order of molecules or ions should be predicted in the following way:

**Ex. H<sub>2</sub>** (number of electrons < 14) : Electronic configuration (E.C.) with MOT  $\sigma_{1s}^2$ , B.O. =  $N_b - N_a / 2 = 2 - 0 / 2 = 1$  (H-H); **H<sub>2</sub><sup>+</sup>**: E.C. with MOT  $\sigma_{1s}^1$ , B.O. =  $N_b - N_a / 2 = 1 - 0 / 2 = 0.5$ ; **H<sub>2</sub><sup>-</sup>**: E.C. with MOT  $\sigma_{1s}^2, \sigma_{1s}^{*1}$ , B.O. =  $N_b - N_a / 2 = 2 - 1 / 2 = 0.5$ .

**He<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}$ , B.O. =  $N_b - N_a / 2 = 2 - 2 / 2 = 0$  (does not exist); **He<sub>2</sub><sup>+</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*1}$ , B.O. =  $N_b - N_a / 2 = 2 - 1 / 2 = 0.5$ .

**Li<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2$ , B.O. =  $N_b - N_a / 2 = 4 - 2 / 2 = 1$ ; **Be<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}$ , B.O. =  $N_b - N_a / 2 = 4 - 4 / 2 = 0$  (does not exist); **B<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^1, \pi_{2py}^1$  (**Fig.4.22**), bond order =  $N_b - N_a / 2 = 6 - 4 / 2 = 1$  (B-B); **C<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2$ , bond order =  $N_b - N_a / 2 = 8 - 4 / 2 = 2$  (C=C).

**N<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2$ , bond order =  $N_b - N_a / 2 = 10 - 4 / 2 = 3$  (N≡N); **N<sub>2</sub><sup>+</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^1$ , bond order =  $N_b - N_a / 2 = 9 - 4 / 2 = 2.5$ ; **N<sub>2</sub><sup>-</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2, \pi_{2px}^{*1}$ , bond order =  $N_b - N_a / 2 = 10 - 5 / 2 = 2.5$ ; **N<sub>2</sub><sup>2-</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2, \pi_{2px}^{*1}, \pi_{2py}^{*1}$ , bond order =  $N_b - N_a / 2 = 10 - 6 / 2 = 2$ .

**O<sub>2</sub>** (number of electrons > 14): E.C. of O<sub>2</sub> is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*1}, \pi_{2py}^{*1}$  (**Fig.4.23**), B.O. =  $N_b - N_a / 2 = 10 - 6 / 2 = 2$  (O=O); **O<sub>2</sub><sup>+</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*1}$ , B.O. =  $N_b - N_a / 2 =$

$10-5/2 = 2.5$ ; **O<sub>2</sub><sup>-</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*1}$ , B.O. =  $N_b - N_a / 2 = 10-7/2 = 1.5$ ;

**O<sub>2</sub><sup>2-</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*2}$ , B.O. =  $N_b - N_a / 2 = 10-8/2 = 1$ .

**F<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*2}$ , B.O. =  $N_b - N_a / 2 = 10-8/2 = 1$  (F-F).

**Ne<sub>2</sub>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*2}, \sigma_{2pz}^{*2}$ , B.O. =  $N_b - N_a / 2 = 10-10/2 = 0$  (does not exist).

**CN** (number of electrons < 14): E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^1$ , bond order =  $N_b - N_a / 2 = 9-4/2 =$

$2.5$ ; **CN<sup>-</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2$ , bond order =  $N_b - N_a / 2 = 10-4/2 = 3$ .

**NO** (number of electrons > 14): E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*1}$ , B.O. =  $N_b - N_a / 2 = 10-5/2$

$= 2.5$ ; **NO<sup>+</sup>**: E.C. is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2$ , B.O. =  $N_b - N_a / 2 = 10-4/2 = 3$ .

## B. Prediction of bond order by the innovative method:

By using innovative mnemonics prediction of bond order of B<sub>2</sub> (total electrons = 10) and O<sub>2</sub> (total electrons = 16) is described below:

**Bond order of B<sub>2</sub>**: B<sub>2</sub> having total number of electrons =10 (total number of electrons, n=10), therefore, it falls in the range (6-14) electrons, for which, as per innovative method, bond order =  $18 - n / 2 = 18 - 10 / 2 = 1$  (B-B).

**Bond order of O<sub>2</sub>**: O<sub>2</sub> having total number of electrons =16 (total number of electrons, n=16), therefore, it falls in the range (14-20) electrons, for which, as per innovative method, bond order =  $20 - n / 2 = 20 - 16 / 2 = 2$  (O=O).

So, with the help of innovative mnemonics, bond order of diatomic species can easily be calculated only from its total number of electrons without drawing a molecular orbital diagram in a time economic method. Adequate examples on the prediction of bond order of homo and heteronuclear diatomic molecules or ions having the total number of electrons fall in the range (1-20) without molecular orbital theory have been explored in **Table 4.4**.

## APPLICATIONS OF BOND ORDER IN CHEMICAL EDUCATION:

### 1. Order of bond properties (bond length, bond Strength, bond dissociation energy, bond energy, ionization energy, thermal stability, reactivity, and vibrational frequency) from bond order value:

From bond order, different parameters like bond length, bond Strength, bond dissociation energy, bond energy, ionization energy, thermal stability, and reactivity can also be evaluated in the following manner:

i) Bond order (B.O.)  $\propto$  1/Bond length or Bond distance ii) B.O.  $\propto$  Bond strength iii) B.O.  $\propto$  Bond dissociation energy iv) B.O.  $\propto$  Bond Energy v) B.O.  $\propto$  Ionization Energy vi) B.O.  $\propto$  1/Reactivity vii) B.O.  $\propto$  Thermal Stability viii) B.O.  $\propto$  vibrational frequency

By knowing the bond order value from the above discussed innovative mnemonics and thus by using the above relations of different parameters with bond order, students and educators can easily be evaluated the increasing or decreasing order of bond length, bond Strength, bond dissociation energy, bond energy, ionization energy, thermal stability and reactivity of different diatomic species.

**Ex.** Bond order values of  $O_2$ ,  $O_2^-$ ,  $O_2^{2-}$ ,  $O_2^+$  and  $O_2^{2+}$  are 2.0, 1.5, 1.0, 2.5 and 3.0 respectively, therefore, decreasing order of their bond length, bond Strength, bond dissociation energy, bond energy, ionization energy, thermal stability, reactivity, and vibrational frequency are  $O_2^{2+}$  (3.0)  $>$   $O_2^+$  (2.5)  $>$   $O_2$  (2.0)  $>$   $O_2^-$  (1.5)  $>$   $O_2^{2-}$  (1.0) and decreasing order of bond length and reactivity are  $O_2^{2-}$  (1.0)  $>$   $O_2^-$  (1.5)  $>$   $O_2$  (2.0)  $>$   $O_2^+$  (2.5)  $>$   $O_2^{2+}$  (3.0).

## 2. Order of stability and reactivity of cationic and anionic species of the same element having same bond order:

When bond order of cationic ( $X_2^+$ ) and anionic species ( $X_2^-$ ) is same for the same element ( $X_2$ ), then anionic species ( $X_2^-$ ) will be much more reactive and least stable than cationic species ( $X_2^+$ ). This is due to the increasing number of electrons in higher energetic antibonding molecular orbital (ABMO) in case of anionic species ( $X_2^-$ ) than that of cationic species ( $X_2^+$ ).

**Ex.a.** Bond order of  $N_2^+$  and  $N_2^-$  is 2.5, then, their reactivity order will be  $N_2^- > N_2^+$  and stability order of will be  $N_2^+ > N_2^-$ .

**Ex.b.** Bond order of  $H_2^+$  and  $H_2^-$  is 0.5, then, their reactivity order will be  $H_2^- > H_2^+$  and stability order of will be  $H_2^+ > H_2^-$ .

## PROBLEMS ON BOND ORDER: (Implementation of Bond-Order Mnemonics to Solve Problems in Competitive Exams)

**Q.1. Which one of these will have the highest bond order? (NEET 2018)**

a)  $CN^+$     b.  $CN^-$     c.  $NO$     d.  $CN$

Ans: b.  $CN^-$  (Total electrons  $n = 6 + 7 + 1 = 14$ , B.O. =  $|8 - n| / 2 = |8 - 14| / 2 = 3$ )

**Q.2. According to molecular orbital theory, which of the following will not be a viable molecule? (JEEMAIN 18)**

- a)  $\text{He}_2^{2+}$  b)  $\text{He}_2^+$  c)  $\text{H}_2^-$  d)  $\text{H}_2^{2-}$

Ans: d)  $\text{H}_2^{2-}$  (Total electrons  $n = 4$ , B.O. =  $(4 - n) / 2 = (4 - 4) / 2 = 0$ , i.e. Does not exist)

**Q.3. Which one of the following pairs of species have the same bond order? (NEET 2017)**

- a)  $\text{O}_2$ ,  $\text{NO}^+$  b)  $\text{CN}^-$ ,  $\text{CO}$  c)  $\text{N}_2$ ,  $\text{O}_2^-$  d)  $\text{CO}$ ,  $\text{NO}$

Ans: (b)  $\text{CN}^-$  and  $\text{CO}$  both having B.O. 3.0 w.r.t. total electrons 14.

**Q.4. Decreasing order of stability of  $\text{O}_2$ ,  $\text{O}_2^-$ ,  $\text{O}_2^+$  and  $\text{O}_2^{2-}$  is (NEET 2015)**

- a)  $\text{O}_2^{2-} > \text{O}_2^- > \text{O}_2 > \text{O}_2^+$  b)  $\text{O}_2 > \text{O}_2^+ > \text{O}_2^{2-} > \text{O}_2^-$  c)  $\text{O}_2^- > \text{O}_2^{2-} > \text{O}_2^+ > \text{O}_2$  d)  $\text{O}_2^+ > \text{O}_2 > \text{O}_2^- > \text{O}_2^{2-}$

Ans: (d)  $\text{O}_2^+$  (2.5)  $>$   $\text{O}_2$  (2.0)  $>$   $\text{O}_2^-$  (1.5)  $>$   $\text{O}_2^{2-}$  (1.0) (B.O.  $\propto$  Stability)

**Q.5. In which of the following pairs of molecules / ions both species are not likely to exist?**

- a)  $\text{H}_2^+$ ,  $\text{He}_2^{2-}$  b)  $\text{H}_2^-$ ,  $\text{He}_2^{2-}$  c)  $\text{H}_2^{2+}$ ,  $\text{He}_2$  d)  $\text{H}_2^-$ ,  $\text{He}_2^{2+}$  (JEE MAIN 2013)

Ans: (c) (B.O. of  $\text{He}_2 = 0$ ) (species having zero or negative bond order do not exist)

**Q.6. Using MOT, predict which of the following species has the shortest bond length?**

- a)  $\text{O}_2^{2+}$  b)  $\text{O}_2^+$  c)  $\text{O}_2^-$  d)  $\text{O}_2^{2-}$  (AIEEE-2009)

Ans: (a) B.O. of  $\text{O}_2^{2+} = 3.0$ ; B.O.  $\propto$  1/Bond length

**Q.7. The molecule / ion having bond order 2.5 is (S.T.P.G.T. 2017)**

- a)  $\text{Li}_2^+$  b)  $\text{F}_2^+$  c)  $\text{O}_2^+$  d)  $\text{C}_2$

Ans: (c) ( $\text{O}_2^+ = 2.5$ )

**Q.8. Using MO theory, predict which of the following species has the shortest bond length ?**

- a)  $\text{O}_2^{2+}$  b)  $\text{O}_2^+$  c)  $\text{O}_2^-$  d)  $\text{O}_2^{2-}$  (AIEEE 2009)

Ans: a)  $\text{O}_2^{2+}$  (B.O. = 3, B.O.  $\propto$  1/ bond length)

**Q.9. Stability of the species increases in the order (JEE MAIN 2013)**

- a)  $\text{Li}_2 < \text{Li}_2^+ < \text{Li}_2^-$  b)  $\text{Li}_2^- < \text{Li}_2^+ < \text{Li}_2$  c)  $\text{Li}_2 < \text{Li}_2^- < \text{Li}_2^+$  d)  $\text{Li}_2^- < \text{Li}_2 < \text{Li}_2^+$

Ans: b.  $\text{Li}_2^- < \text{Li}_2^+ < \text{Li}_2$

( $\text{Li}_2 = \text{B.O.} = 1$ ,  $\text{Li}_2^+$  &  $\text{Li}_2^-$  B.O. = 0.5; Bond order  $\propto$  stability, but when bond order be same then cationic species will have higher stability than anionic species due to increase in electron in higher energetic ABMO in anionic species)

**Q.10. Among the following species, the order of first ionization energy ( $\text{IE}_1$ ) is**

- a)  $\text{O}_2 < \text{O}_2^+ < \text{O}_2^-$  b)  $\text{O}_2^+ < \text{O}_2^- < \text{O}_2$  c)  $\text{O}_2^- < \text{O}_2 < \text{O}_2^+$  d)  $\text{O}_2 < \text{O}_2^- < \text{O}_2^+$

Ans: c.  $\text{O}_2^- < \text{O}_2 < \text{O}_2^+$  -  $\text{IE}_1$  (Bond order  $\propto$   $\text{IE}_1$ ; Bond order trend is  $1.5 < 2.0 < 2.5$ )

**Q.11. Which of the following is the correct order of their stability ?**

- a.  $\text{CN} < \text{NO}^+ < \text{NO}^-$    b.  $\text{NO}^- < \text{CN} < \text{NO}^+$    c.  $\text{NO}^+ < \text{CN} < \text{NO}^-$    d.  $\text{CN} < \text{NO}^- < \text{NO}^+$

Ans: b.  $\text{NO}^-$  (2.0) <  $\text{CN}$  (2.5) <  $\text{NO}^+$  (3.0) - stability (Bond order  $\propto$  stability)

**Q.12. In which case bond order increases ?**

- a.  $\text{O}_2$  changes to  $\text{O}_2^+$    b.  $\text{N}_2$  changes to  $\text{N}_2^+$    c.  $\text{NO}$  changes to  $\text{NO}^-$    d. In all cases

Ans: a.  $\text{O}_2$  changes to  $\text{O}_2^+$  (bond order increases from 2.0 to 2.5)

**Q.13. Which of the following is the correct order of their stability ?**

- a.  $\text{N}_2 > \text{N}_2^+ > \text{N}_2^-$    b.  $\text{N}_2 > \text{N}_2^- > \text{N}_2^+$    c.  $\text{N}_2^+ > \text{N}_2 > \text{N}_2^-$    d. None of these

Ans: a.  $\text{N}_2 > \text{N}_2^+ > \text{N}_2^-$  (Bond order of  $\text{N}_2 = 3.0$ ,  $\text{N}_2^+$  &  $\text{N}_2^- = 2.5$ ; Bond order  $\propto$  stability)

**Q.14. Which of the following is non-existent according to molecular orbital theory ?**

- a.  $\text{H}_2^-$    b.  $\text{O}_2^-$    c.  $\text{He}_2$    d.  $\text{O}_2^+$

Ans:  $\text{He}_2$  (B.O. = 0)

**Q.15. The molecular species having highest bond order is**

- a.  $\text{O}_2$    b.  $\text{O}_2^-$    c.  $\text{O}_2^+$    d.  $\text{O}_2^{2-}$

Ans: c.  $\text{O}_2^+$  (B.O. = 2.5)

**Q.16.  $\text{N}_2$  and  $\text{O}_2$  are converted into mono cations  $\text{N}_2^+$  and  $\text{O}_2^-$  respectively. Which is wrong ?**

- a. In  $\text{N}_2^+$ , the N-N bond weakens   b. In  $\text{O}_2^+$ , the O-O bond increases   c. In  $\text{O}_2^+$ , Paramagnetism decreases  
d.  $\text{N}_2^+$ , becomes diamagnetic

Ans: d.  $\text{N}_2^+$ , because,  $\text{N}_2^+$  becomes paramagnetic not diamagnetic

**Q.17. The calculated bond order in  $\text{H}_2^-$  ion is**

- a. 0   b. 1/2   c. -1/2   d. 1

Ans: b. 1/2

**Q.18. Which is the correct sequence of bond order?**

- a.  $\text{O}_2^+ > \text{O}_2^- > \text{O}_2$    b.  $\text{O}_2 > \text{O}_2^- > \text{O}_2^+$    c.  $\text{O}_2^+ > \text{O}_2 > \text{O}_2^-$    d.  $\text{O}_2^- > \text{O}_2^+ > \text{O}_2$

Ans: c.  $\text{O}_2^+ > \text{O}_2 > \text{O}_2^-$  ( B.O. 2.5 > 2.0 > 1.5)

**Q.19. The molecule having bond order 3 is**

- a.  $\text{H}_2$    b.  $\text{N}_2$    c.  $\text{O}_2$    d.  $\text{He}_2^+$

Ans: b.  $\text{N}_2$  (B.O. = 3)

**Q.20. The relationship between the dissociation energy of  $\text{N}_2$  and  $\text{N}_2^+$  is**



- a. Dissociation energy of  $N_2 =$  dissociation energy of  $N_2^+$   
 b. Dissociation energy of  $N_2$  can either be lower or higher than the dissociation energy of  $N_2^+$   
 c. Dissociation energy of  $N_2 >$  dissociation energy of  $N_2^+$   
 d. Dissociation energy of  $N_2 <$  dissociation energy of  $N_2^+$

Ans: c. Dissociation energy of  $N_2 >$  dissociation energy of  $N_2^+$  (B.O. of  $N_2$  is 3.0 and that of  $N_2^+$  is 2.5)

**Q.21. An antibonding molecular orbital is formed by**

- a. Addition of atomic orbitals    b. Subtraction of atomic orbitals    c. Multiplication of atomic orbitals  
 d. None of these.

Ans: b. Subtraction of atomic orbitals gives rise to Antibonding molecular orbitals

**Q.22. A bonding molecular orbital is formed by**

- a. Addition of atomic orbitals    b. Subtraction of atomic orbitals    c. Division of atomic orbitals  
 d. None of these.

Ans: a. Addition of atomic orbitals gives rise to bonding molecular orbitals

**Q.23. The bond order of  $O_2^-$  is**

- a.0.5    b.1.5    c.3.5    d.2.5

Ans: b.1.5

**Q.24. The number of antibonding electron pairs on  $O_2^{2-}$  molecular ion on the basis of MOT is**

- a.4    b.3    c.2    d.5

Ans: a.4 (E.C. of  $O_2^{2-}$  is  $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2p_z}^2, \pi_{2p_x}^2, \pi_{2p_y}^2, \pi_{2p_x}^{*2}, \pi_{2p_y}^{*2}$ )

**Q.25. The common features among the species  $CN^-$ ,  $CO$  and  $NO^+$  are**

- a. Bond order 3 and isoelectronic    b. Bond order 3 and weak field ligands  
 c. Bond order 3 and  $\pi$ -acceptors    d. Isoelectronic and weak field ligands

Ans: a. Bond order 3 and isoelectronic (All having 14 electrons and 3 B.O.)

**Q.26. Two  $sp^3$  hybridized carbons are present in which of the following compounds?**

- a.  $CH_3CH=CH_2$     b.  $CH_3CH_2OH$     c.  $CH_3CHO$     d.  $CH_3COOH$

Ans: b.  $CH_3CH_2OH$  (Both carbon atoms in ethanol are surrounded by 4  $\sigma$  bonds and hence are in  $sp^3$  hybridized)

**Q.27. Match column I with column II and select the correct answer using the code given below:**

**Column I (Molecule/Ion)**

**Column II (Molecular Geometry)**

A. $\text{HgCl}_2$	1. Tetrahedral
B. $\text{NH}_4^+$	2. Trigonal bipyramidal
C. $\text{SF}_6$	3. Linear
D. $\text{PCl}_5$	4. Octahedral

A	B	C	D
a. 4	3	2	1
b. 3	1	4	2
c. 3	2	1	4
d. 2	3	4	1

Ans: b.

**Q.28. Which of the following statements is incorrect?**

- a. A double bond is stronger than a single bond      b. A double bond is shorter than a single bond  
 c.  $\pi$  bond is stronger bond      d.  $\pi$  bond does not affect the shape of the molecule

Ans: c.  $\pi$  bond is a weak bond

**Q.29. How many  $\sigma$  and  $\pi$  bonds are present in  $\text{C}_2\text{H}_4$ ?**

- a. 5 & 2      b. 5 & 1      c. 4 & 3      d. 4 & 1

Ans: b. 5 & 1 (5 $\sigma$  bonds and 1 $\pi$  bond)

**Q.30. In  $\text{NO}_3^-$  ion, the number of lone pair and bond pairs of electrons on nitrogen are**

- a. 4,0      b. 0,4      c. 2,3      d. 0,5

Ans: b. 0,4 (In  $\text{HNO}_3$  nitrogen is surrounded by one coordinate bond with O, one double bond O and one single bond with -O-H)

**Q.31. Which of the following pair has an identical bond order?**

- a.  $\text{CN}^-$  &  $\text{O}_2^-$       b.  $\text{O}_2^-$  &  $\text{CN}^+$       c.  $\text{CN}^+$  &  $\text{CN}^-$       d.  $\text{CN}^-$  &  $\text{NO}^+$

Ans: d.  $\text{CN}^-$  &  $\text{NO}^+$  (Both having 14 electrons, B.O. = 3)

**Q.32. Which of the following angle corresponds to  $\text{sp}^3$  hybridization?**

- a.  $180^\circ$       b.  $120^\circ$       c.  $109^\circ 28'$       d.  $90^\circ$

Ans: c.  $109^\circ 28'$

**Q.33. Which of the following is not linear?**

- a. HF      b.  $\text{H}_2\text{S}$       c.  $\text{H}_2$       d. HI

Ans: b.  $\text{H}_2\text{S}$  (Bent or angular shape,  $\text{sp}^3$ , LP = 2, BP = 2)

**Q.34. The hybridization of P in  $\text{PCl}_5$  is**

a.  $\text{sp}^3$       b.  $\text{sp}^3\text{d}$       c.  $\text{sp}^3\text{d}^2$       d.  $\text{sp}^2$

Ans: b.  $\text{sp}^3\text{d}$  (LP=0, BP = 5)

**Q.35. Which one of the following has the regular tetrahedral structure?**

a.  $\text{XeF}_4$       b.  $\text{SF}_4$       c.  $\text{BF}_4^-$       d.  $[\text{Ni}(\text{CN})_4]^{2-}$

Ans: c.  $\text{BF}_4^-$  (BP = 4 & LP = 0)

**Q.36. Arrange the following molecules in order of increasing fundamental vibrational frequencies (NET 2018)**

a)  $\text{O}_2^{2-} < \text{O}_2^- < \text{O}_2 < \text{O}_2^+$     b)  $\text{O}_2 < \text{O}_2^+ < \text{O}_2^- < \text{O}_2^{2-}$     c)  $\text{O}_2^{2-} < \text{O}_2^- < \text{O}_2^+ < \text{O}_2$     d) a)  $\text{O}_2^+ < \text{O}_2 < \text{O}_2^- < \text{O}_2^{2-}$

Ans: a)  $\text{O}_2^{2-} < \text{O}_2^- < \text{O}_2 < \text{O}_2^+$  (B.O. order is  $1 < 1.5 < 2 < 2.5$ ; B.O.  $\propto$  vibrational frequencies)

## Conclusion

It may be expected that these time economic innovative mnemonics, described in chapter 4, will help students, scholars and educators in chemical education at Undergraduate, Senior Undergraduate and Post-Graduate level to predict the bond order of homo and heteronuclear molecules or ions and its related properties without drawing electronic configuration of diatomic species with MOT. Experiments, *in vitro*, on 100 students, showed that, by using these innovative formulae, students can save up to 10-15 minutes' time in the examination hall to solve different problems regarding bond order and its related properties in inorganic chemistry. On the basis of this, I can strongly recommend using these time economic innovative mnemonics in inorganic chemistry.

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